```
=> file hcaplus
FILE 'HCAPLUS' ENTERED AT 15:23:11 ON 17 JUL 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)
```



```
FILE COVERS 1907 - 17 Jul 2007  VOL 147 ISS 4
FILE LAST UPDATED: 16 Jul 2007  (20070716/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.
'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

=> d que nos l44
L40         439 SEA FILE=HCAPLUS ABB=ON  PLU=ON  SAVAGE P?/AU
L41          85 SEA FILE=HCAPLUS ABB=ON  PLU=ON  BENDELAC A?/AU
L42         103 SEA FILE=HCAPLUS ABB=ON  PLU=ON  TEYTON L?/AU
L43          20 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L40 AND L41 AND L42
L44           5 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L43 AND (1840-2003)/PRY,
                 PY,AY


=> d ibib ed abs l44 1-5

L44  ANSWER 1 OF 5  HCAPLUS  COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:         2004:927222  HCAPLUS
DOCUMENT NUMBER:          141:350362
TITLE:                    Synthesis and NKT Cell Stimulating Properties of
                          Fluorophore- and Biotin-Appended
                          6''-Amino-6''-deoxy-galactosylceramides
INVENTOR(S):              Savage, Paul B.; Bendelac,
                          Albert; Teyton, Luc
PATENT ASSIGNEE(S):       Brigham Young University, USA
SOURCE:                   PCT Int. Appl., 52 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.           KIND   DATE        APPLICATION NO.        DATE
     ---------------      ----   --------    --------------------
     --------
     WO 2004094444         A1    20041104    WO 2003-US8530
                                                                   200303
                                                                   20
                                                <--
```

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

CA 2519568	A1	20041104	CA 2003-2519568	200303 20
			<--	
AU 2003225891	A1	20041119	AU 2003-225891	200303 20
			<--	
EP 1611147	A1	20060104	EP 2003-816701	200303 20
			<--	

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK

US 2006264382	A1	20061123	US 2005-550165	200509 20
			<--	
PRIORITY APPLN. INFO.:			WO 2003-US8530 W	200303 20
			<--	

OTHER SOURCE(S): MARPAT 141:350362
ED Entered STN: 04 Nov 2004
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB α-Galactosylceramides I, wherein R1 is H, substituted sulfonyl; R1R2 together form heterocycle; R2 is H; R3-R7 are independently H, alkyl, aralkyl, acyl; R8 is (CH2)xMe; x is 1-100; R9 is alkyl, are potent stimulators of human T cells. Stimulation occurs through binding of the glycolipids by CD1d, presentation to T cells, and formation of a CD1D-glycolipid-T cell receptor complex. To facilitate the elucidation of the structural features of glycolipids necessary for T cell stimulation, α-galactosylceramides have been prepared with small mols. appended at the C6 position of the sugar. The appended mols. do not significantly influence the abilities of the glycolipids to stimulate T cells. Thus, galactosylceramide II was prepared and tested in mice in stimulating NKT cells.

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L44 ANSWER 2 OF 5 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:306445 HCAPLUS
DOCUMENT NUMBER: 138:400350
TITLE: The Paradox of Immune Molecular Recognition of α-Galactosylceramide: Low Affinity, Low Specificity for CD1d, High Affinity for αβ TCRs
AUTHOR(S): Cantu, Carlos, III; Benlagha, Kamel; **Savage, Paul B.**; **Bendelac, Albert**; **Teyton, Luc**
CORPORATE SOURCE: Department of Immunology, The Scripps Research Institute, La Jolla, CA, 92037, USA
SOURCE: Journal of Immunology (**2003**), 170(9), 4673-4682
CODEN: JOIMA3; ISSN: 0022-1767
PUBLISHER: American Association of Immunologists
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 22 Apr 2003
AB CD1 resembles both class I and class II MHC but differs by the important aspect of presenting lipid/glycolipids, instead of peptides, to T cells. Biophys. studies of lipid/CD1 interactions have been limited, and kinetics of binding are in contradiction with functional studies. We have revisited this issue by designing new assays to examine the loading of CD1 with lipids. As expected for hydrophobic interactions, binding affinity was not high and had limited specificity. Lipid critical micelle concentration set the limitation to these studies. Once loaded onto CD1d, the recognition of glycolipids by αβ T cell receptor was studied by surface plasmon resonance using soluble Vα14-Vβ8.2 T cell receptors. The Vα14 Jα18 chain could be paired with NK1.1 cell-derived Vβ chain, or any Vβ8 chain, to achieve high affinity recognition of α-galactosylceramide. Biophys. anal. indicated little effect of temperature or ionic strength on the binding interaction, in contrast to what has been seen in peptide/MHC-TCR studies. This suggests that there is less accommodation made by this TCR in recognizing α-galactosylceramide, and it can be assumed that the most rigid part of the Ag, the sugar moiety, is critical in the interaction.
REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L44 ANSWER 3 OF 5 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:318756 HCAPLUS
TITLE: Lipid presentation by CD1: the short and the long lipid story
AUTHOR(S): **Bendelac, A.**; **Teyton, L.**; **Savage, P. B.**
CORPORATE SOURCE: Department of Molecular Biology, Princeton University, Princeton, NJ, 08544, USA
SOURCE: Nature Immunology (**2002**), 3(5), 421-422
CODEN: NIAMCZ; ISSN: 1529-2908
PUBLISHER: Nature America Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 29 Apr 2002
AB Unavailable

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L44 ANSWER 4 OF 5 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:207112 HCAPLUS
DOCUMENT NUMBER: 136:369933
TITLE: Synthesis and NKT Cell Stimulating Properties of Fluorophore- and Biotin-Appended 6''-Amino-6''-deoxy-galactosylceramides
AUTHOR(S): Zhou, Xiao-Ti; Forestier, Claire; Goff, Randal D.; Li, Chunhong; **Teyton, Luc**; **Bendelac, Albert**; **Savage, Paul B.**
CORPORATE SOURCE: Department of Chemistry and Biochemistry, Brigham Young University, Provo, UT, 84602, USA
SOURCE: Organic Letters (**2002**), 4(8), 1267-1270
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 136:369933
ED Entered STN: 20 Mar 2002
AB α-Galactosylceramides are potent stimulators of human T cells. Stimulation occurs through binding of the glycolipids by CD1d, presentation to T cells, and formation of a CD1D-glycolipid-T cell receptor complex. To facilitate the elucidation of the structural features of glycolipids necessary for T cell stimulation, α-galactosylceramides have been prepared with small mols. appended at the C6 position of the sugar. The appended mols. do not significantly influence the abilities of the glycolipids to stimulate T cells.
REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L44 ANSWER 5 OF 5 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:43462 HCAPLUS
DOCUMENT NUMBER: 136:230865
TITLE: Multiple defects in antigen presentation and T cell development by mice expressing cytoplasmic tail-truncated CD1d
AUTHOR(S): Chiu, Ya-Hui; Park, Se-Ho; Benlagha, Kamel; Forestier, Claire; Jayawardena-Wolf, Jayanthi; **Savage, Paul B.**; **Teyton, Luc**; **Bendelac, Albert**
CORPORATE SOURCE: Department of Molecular Biology, Princeton University, Princeton, NJ, 08544, USA
SOURCE: Nature Immunology (**2002**), 3(1), 55-60
CODEN: NIAMCZ; ISSN: 1529-2908
PUBLISHER: Nature America Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 17 Jan 2002
AB For members of the CD1 family of β2-microglobulin-associated lipid-presenting mols., tyrosine-based motifs in the cytoplasmic tail and invariant chain (Ii) govern glycoprotein trafficking through endosomal compartments. Little is known about the intracellular pathways of CD1 trafficking and antigen presentation.

However, in vitro studies with cells transfected with mutant CD1 that had a truncated cytoplasmic tail have suggested a role for these tyrosine motifs in some, but not all, antigenic systems. By introducing a deletion of the tyrosine motif into the germ line, and through homologous recombination in embryonic stem cells, we now describe knock-in mice with the CD1d cytoplasmic tail deleted. Despite adequate surface CD1d expression and the presence of Ii, these mutant mice showed multiple and selective abnormalities in intracellular trafficking, antigen presentation and T cell development, demonstrating the critical functions of the CD1d cytoplasmic tail motif in vivo.

REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d his nofile

(FILE 'HOME' ENTERED AT 12:09:06 ON 17 JUL 2007)

FILE 'HCAPLUS' ENTERED AT 12:09:20 ON 17 JUL 2007
E US20060264382/PN
L1 1 SEA ABB=ON PLU=ON US2006264382/PN
SEL RN

FILE 'REGISTRY' ENTERED AT 12:09:41 ON 17 JUL 2007
L2 19 SEA ABB=ON PLU=ON (158021-47-7/BI OR 205371-68-2/BI OR 217176-82-4/BI OR 35013-72-0/BI OR 424823-18-7/BI OR 424823-19-8/BI OR 424823-20-1/BI OR 424823-22-3/BI OR 424823-23-4/BI OR 424823-24-5/BI OR 424823-25-6/BI OR 424823-26-7/BI OR 424823-27-8/BI OR 424823-28-9/BI OR 424823-29-0/BI OR 424823-30-3/BI OR 4711-00-6/BI OR 605-65-2/BI OR 88714-17-4/BI)

FILE 'HCAPLUS' ENTERED AT 12:09:50 ON 17 JUL 2007
L3 1 SEA ABB=ON PLU=ON L1 AND L2

FILE 'REGISTRY' ENTERED AT 12:23:36 ON 17 JUL 2007
L36 STRUCTURE
L37 0 SEA SSS SAM L36
L38 17 SEA SSS FUL L36
SAV L38 KRI165/A

FILE 'HCAPLUS' ENTERED AT 15:11:35 ON 17 JUL 2007
L39 8 SEA ABB=ON PLU=ON L38
L40 439 SEA ABB=ON PLU=ON SAVAGE P?/AU
L41 85 SEA ABB=ON PLU=ON BENDELAC A?/AU
L42 103 SEA ABB=ON PLU=ON TEYTON L?/AU
L43 20 SEA ABB=ON PLU=ON L40 AND L41 AND L42
L44 5 SEA ABB=ON PLU=ON L43 AND (1840-2003)/PRY,PY,AY
L45 6 SEA ABB=ON PLU=ON L39 NOT L44

FILE 'HCAPLUS' ENTERED AT 15:23:11 ON 17 JUL 2007
D QUE NOS L44
D IBIB ED ABS L44 1-5

=> file reg
FILE 'REGISTRY' ENTERED AT 15:23:37 ON 17 JUL 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 16 JUL 2007 HIGHEST RN 942468-13-5
DICTIONARY FILE UPDATES: 16 JUL 2007 HIGHEST RN 942468-13-5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

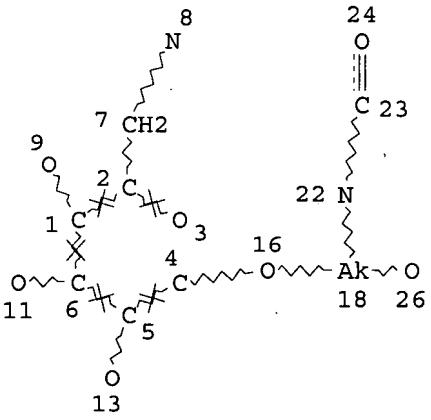
TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=> d stat que l38
L36 STR



NODE ATTRIBUTES:
NSPEC IS RC AT 3
NSPEC IS RC AT 4
NSPEC IS RC AT 8
DEFAULT MLEVEL IS ATOM
MLEVEL IS CLASS AT 18
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 17

STEREO ATTRIBUTES: NONE
L38 17 SEA FILE=REGISTRY SSS FUL L36

100.0% PROCESSED 332123 ITERATIONS 17 ANSWERS
SEARCH TIME: 00.00.08

```
=> file hcaplus
FILE 'HCAPLUS' ENTERED AT 15:23:48 ON 17 JUL 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)
```



```
FILE COVERS 1907 - 17 Jul 2007  VOL 147 ISS 4
FILE LAST UPDATED: 16 Jul 2007  (20070716/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.
'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

=> d que nos l45
L36             STR
L38          17 SEA FILE=REGISTRY SSS FUL L36
L39           8 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L38
L40         439 SEA FILE=HCAPLUS ABB=ON  PLU=ON  SAVAGE P?/AU
L41          85 SEA FILE=HCAPLUS ABB=ON  PLU=ON  BENDELAC A?/AU
L42         103 SEA FILE=HCAPLUS ABB=ON  PLU=ON  TEYTON L?/AU
L43          20 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L40 AND L41 AND L42
L44           5 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L43 AND (1840-2003)/PRY,
                PY,AY
L45           6 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L39 NOT L44


=> d ibib ed abs hitstr l45 1-6

L45  ANSWER 1 OF 6  HCAPLUS  COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:         2007:463101  HCAPLUS
DOCUMENT NUMBER:          146:440188
TITLE:                    Hexosylceramides as adjuvants and their uses in
                          pharmaceutical compositions
INVENTOR(S):              Ebensen, Thomas; Morr, Michael; Guzman, Carlos
                          A.
PATENT ASSIGNEE(S):       GBF Gesellschaft fuer Biotechnologische
                          Forschung Mbh, Germany
SOURCE:                   PCT Int. Appl., 61pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.           KIND   DATE        APPLICATION NO.        DATE
     ---------------      ----   --------    --------------------
```

WO 2007045469 A1 20070426 WO 2006-EP10086
200610
19

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

EP 1776963 A1 20070425 EP 2005-22771
200510
19

R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, MK, YU

PRIORITY APPLN. INFO.: EP 2005-22771 A
200510
19

OTHER SOURCE(S): MARPAT 146:440188

ED Entered STN: 27 Apr 2007

AB The present invention relates to new adjuvants and the uses in pharmaceutical compns., like in vaccines. In particular, the present invention provides new compds. useful as adjuvants for prophylactic and/or therapeutic vaccination in the treatment of infectious diseases, inflammatory diseases, autoimmune diseases, tumors, allergies as well as for the control of fertility in human or animal populations. The compds. are particularly useful not only as systemic, but preferably as mucosal adjuvants. In addition, the invention relates to its uses as active ingredients in pharmaceutical compns.

IT **934480-71-4P**

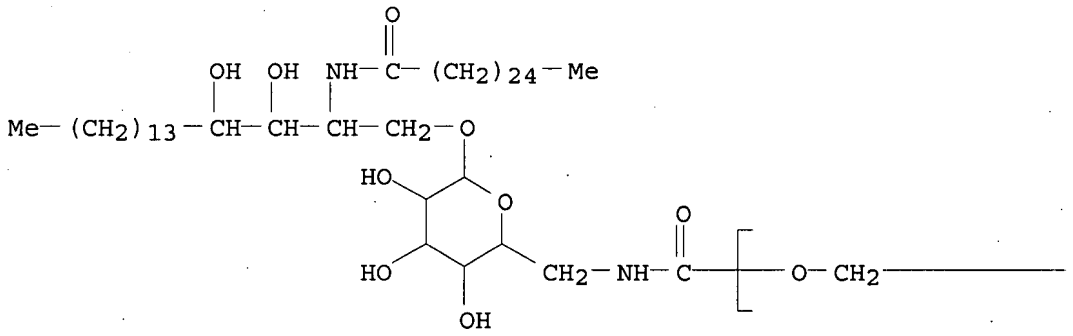
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(hexosylceramides as adjuvants and their use in vaccines)

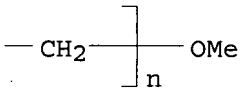
RN 934480-71-4 HCAPLUS

CN Poly(oxy-1,2-ethanediyl), α-hydro-ω-methoxy-, ester with N-[(1S,2S,3R)-1-[[[6-(carboxyamino)-6-deoxy-α-D-galactopyranosyl]oxy]methyl]-2,3-dihydroxyheptadecyl]hexacosanamide (CA INDEX NAME)

PAGE 1-A

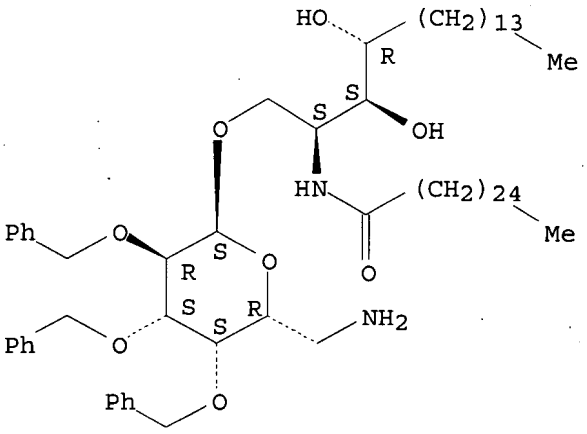


PAGE 1-B



IT **424823-29-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(hexosylceramides as adjuvants and their use in vaccines)
RN 424823-29-0 HCAPLUS
CN Hexacosanamide, N-[(1S,2S,3R)-1-[[[6-amino-6-deoxy-2,3,4-tris-O-(phenylmethyl)-α-D-galactopyranosyl]oxy]methyl]-2,3-dihydroxyheptadecyl]- (CA INDEX NAME)

Absolute stereochemistry.



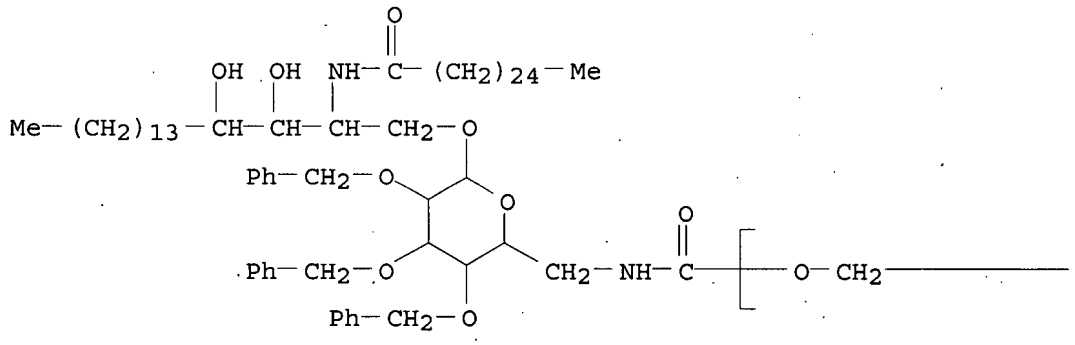
IT **934480-72-5P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(hexosylceramides as adjuvants and their use in vaccines)

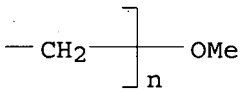
RN 934480-72-5 HCAPLUS

CN Poly(oxy-1,2-ethanediyl), α-hydro-ω-methoxy-, ester with N-[(1S,2S,3R)-1-[[[6-(carboxyamino)-6-deoxy-2,3,4-tris-O-(phenylmethyl)-α-D-galactopyranosyl]oxy]methyl]-2,3-dihydroxyheptadecyl]hexacosanamide (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L45 ANSWER 2 OF 6 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:533879 HCAPLUS

DOCUMENT NUMBER: 145:143203

TITLE: A modified α-galactosyl ceramide for staining and stimulating natural killer T cells

AUTHOR(S): Liu, Yang; Goff, Randal D.; Zhou, Dapeng; Mattner, Jochen; Sullivan, Barbara A.; Khurana, Archana; Cantu, Carlos; Ravkov, Eugene V.; Ibegbu, Chris C.; Altman, John D.; Teyton, Luc; Bendelac, Albert; Savage, Paul B.

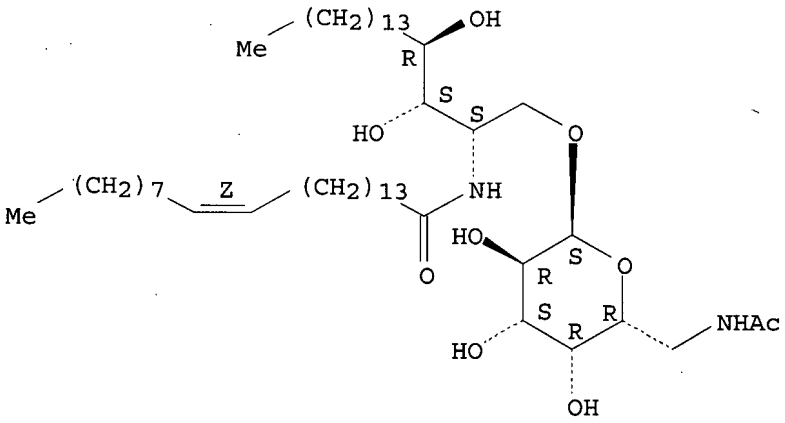
CORPORATE SOURCE: Brigham Young University, Provo, UT, 84602, USA

SOURCE: Journal of Immunological Methods (2006), 312(1-2), 34-39
CODEN: JIMMBG; ISSN: 0022-1759

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 07 Jun 2006
AB CD1d presentation of α-galactosyl ceramides to natural killer T cells has been a focal point of the study of regulatory T cells. KRN7000, an α-galactosyl ceramide originally generated from structure activity studies of antitumor properties of marine sponge glycolipids, is currently the most commonly used agonist ligand and is used to stain NKT cells. However, this glycolipid suffers from poor solubility and availability. The authors have developed an α-galactosyl ceramide with improved solubility over KRN7000 that effectively stains NKT cells, both mouse and human, and stimulates cytokine release at low concns.
IT **898531-99-2**, PBS 57
RL: ARG (Analytical reagent use); PRP (Properties); ANST (Analytical study); USES (Uses)
(α-galactosyl ceramide ligand for staining and stimulation of NK T-cells)
RN 898531-99-2 HCAPLUS
CN 15-Tetracosenamide, N-[(1S,2S,3R)-1-[[[6-(acetylamino)-6-deoxy-α-D-galactopyranosyl]oxy]methyl]-2,3-dihydroxyheptadecyl]-, (15Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

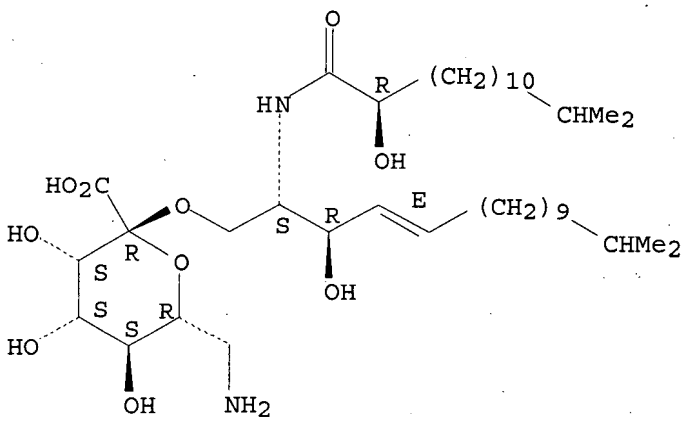


REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L45 ANSWER 3 OF 6 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:523485 HCAPLUS
DOCUMENT NUMBER: 141:257202
TITLE: Phylogeny of the ring-forming bacterium Arcicella aquatica gen. nov., sp. nov. (ex Nikitin et al. 1994), from a freshwater neuston biofilm
AUTHOR(S): Nikitin, Denis I.; Stroempl, Carsten; Oranskaya, M. S.; Abraham, Wolf-Rainer
CORPORATE SOURCE: Institute of Microbiology, Russian Academy of Sciences, Moscow, 117811, Russia
SOURCE: International Journal of Systematic and Evolutionary Microbiology (2004), 54(3), 681-684

CODEN: ISEMF5; ISSN: 1466-5026
PUBLISHER: Society for General Microbiology
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 30 Jun 2004
AB Arcicella aquatica NO-502T, obtained from a neuston film on a freshwater lake and belonging to the phylum Bacteroidetes, is characterized by ring-forming cells. The bacterium is a strict aerobe, with optimal growth between 28 and 30°. Carbohydrates, but no organic acids or amino acids, are used as substrates. The G+C content of strain NO-502T is 34.5 mol%; its genome size is 2.9+109 Da. The genus Arcicella and its type species Arcicella aquatica (type strain NO-502T=LMG 21963T=CIP 107990T) are proposed, and descriptions of this genus and species are given.
IT **251095-67-7**
RL: BSU (Biological study, unclassified); BIOL (Biological study) (phylogeny and biochem. characterization of ring-forming bacterium Arcicella aquatica from a freshwater neuston biofilm based on rDNA sequences and polar lipids)
RN 251095-67-7 HCAPLUS
CN α-D-manno-2-Heptulopyranosidonic acid, (2S,3R,4E)-3-hydroxy-2-[[(2R)-2-hydroxy-13-methyl-1-oxotetradecyl]amino]-15-methyl-4-hexadecenyl 7-amino-7-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L45 ANSWER 4 OF 6 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:132275 HCAPLUS
DOCUMENT NUMBER: 136:356788
TITLE: Regioselective reaction of unprotected sugars with urethane N-carboxyanhydrides for the synthesis of new surfactants
AUTHOR(S): Bellhaouel, Salima; Roumestant, Marie-Louise; Viallefont, Philippe; Martinez, Jean
CORPORATE SOURCE: UMR 5810-CNRS Laboratoire des Amino Acides, Peptides et Proteines, Montpellier, 34095, Fr.
SOURCE: Synthetic Communications (2002), 32(2), 181-187

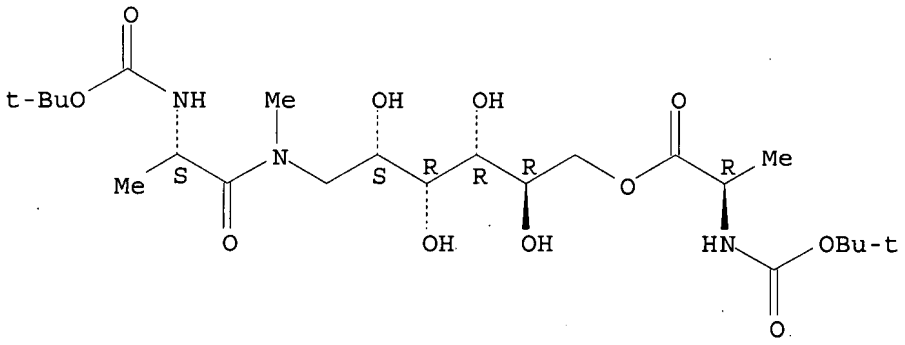
CODEN: SYNCAV; ISSN: 0039-7911
PUBLISHER: Marcel Dekker, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 20 Feb 2002

AB Reaction of urethane N-carboxyanhydrides with unprotected amino sugars was the key step in the synthesis of new trimodular surfactants. Reaction of a 2:1 mixture of N-methylglucamine with the N-BOC derivative of 4-methyl-1,3-oxazoline-2,5-dione in DMF at room temperature gave a 36% yield of N-[(2-BOC-amino)propionyl]-N-methylglucamine.

IT **420132-49-6P 420132-50-9P 420132-51-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(regioselective reaction of unprotected sugars with urethane N-carboxyanhydrides for synthesis of new surfactants)

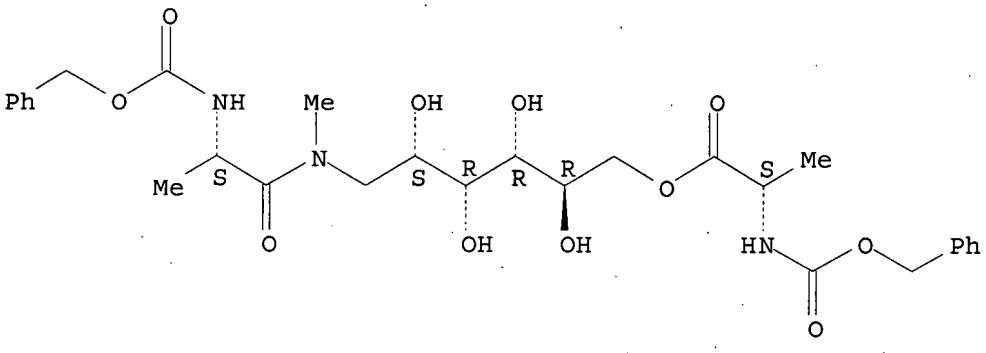
RN 420132-49-6 HCAPLUS
CN L-Alanine, N-[(1,1-dimethylethoxy)carbonyl]-, 6-ester with 1-deoxy-1-[[(2S)-2-[[(1,1-dimethylethoxy)carbonyl]amino]-1-oxopropyl]methylamino]-D-glucitol (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 420132-50-9 HCAPLUS
CN L-Alanine, N-[(phenylmethoxy)carbonyl]-, 6-ester with 1-deoxy-1-[methyl[(2S)-1-oxo-2-[[(phenylmethoxy)carbonyl]amino]propyl]amino]-D-glucitol (9CI) (CA INDEX NAME)

Absolute stereochemistry.

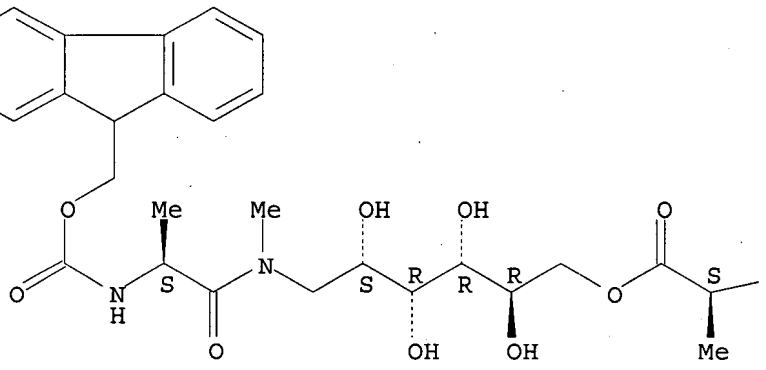


RN 420132-51-0 HCAPLUS
CN L-Alanine, N-[(9H-fluoren-9-ylmethoxy)carbonyl]-, 6-ester with 1-deoxy-1-[[(2S)-2-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-1-

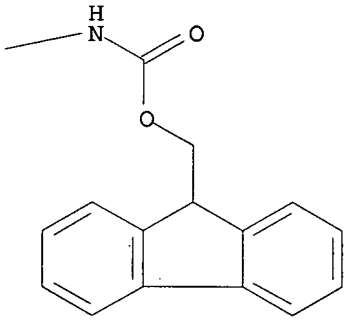
oxopropyl]methylamino]-D-glucitol (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

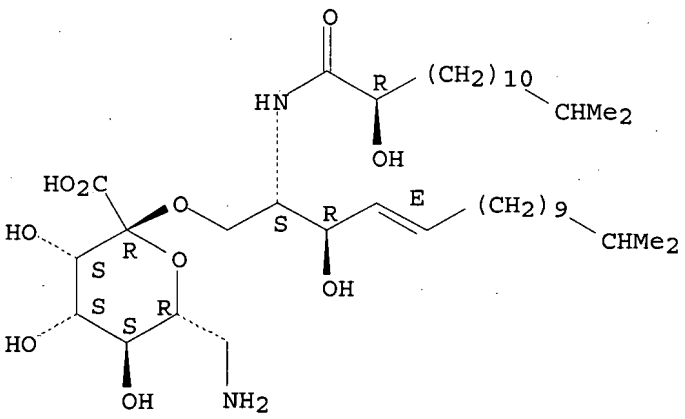
L45 ANSWER 5 OF 6 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1999:584460 HCAPLUS
DOCUMENT NUMBER: 132:1853
TITLE: A novel glycosphingolipid from Gram-negative aquatic bacteria
AUTHOR(S): Batrakov, S. G.; Sheichenko, V. I.; Nikitin, D. I.
CORPORATE SOURCE: Research Centre 'Hydrobios' of Ministry of Health, Moscow, Russia
SOURCE: Biochimica et Biophysica Acta, Molecular and

Cell Biology of Lipids (1999), 1440(2-3), 163-175
CODEN: BBMLFG; ISSN: 1388-1981
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 17 Sep 1999

AB The chloroform-methanol extractable lipids of the Gram-neg. fresh-water bacteria Arcocella aquatica NO-502 and Flectobacillus major FM were found to contain an unusual ninhydrin-pos. glycolipid. It was purified by two-stage silica gel-column chromatog. By the use of IR and 1H-NMR spectroscopy, mass spectrometry and chemical-degradation experiment, the lipid was established to be 1-O-monoglycosyl ceramide, the carbohydrate moiety of which was the α-pyranose-ring form of 7-desoxy-7-amino-D-manno-heptulosonic acid, or 1-hydroxycarbonyl-6-deoxy-6-amino-α-D-mannopyranose. The ceramide portion consisted mainly (by 95% in the A. aquatica glycolipid and 80% in the F. major glycolipid) of 2-N-(2'-D-hydroxy-13'-methyltetradecanoyl)-15-methyl-4(E)-hexadecasphingenine. The minor mol. species differed from the major one only in fatty acid structure. The glycolipid accounted for 8 and 11% of the total lipids extracted from A. aquatica NO-502 and F. major FM cells, resp.

IT **251095-67-7P**
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(novel glycosphingolipid from Gram-neg. aquatic bacteria)
RN 251095-67-7 HCAPLUS
CN α-D-manno-2-Heptulopyranosidonic acid, (2S,3R,4E)-3-hydroxy-2-[[(2R)-2-hydroxy-13-methyl-1-oxotetradecyl]amino]-15-methyl-4-hexadecenyl 7-amino-7-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L45 ANSWER 6 OF 6 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1997:359192 HCAPLUS
DOCUMENT NUMBER: 127:81767

TITLE: Internally quenched fluorogenic, α-helical dimeric peptides and glycopeptides for the evaluation of the effect of glycosylation on the conformation of peptides

AUTHOR(S): Mehta, Seema; Meldal, Morten; Ferro, Vito; Duus, Jens O.; Bock, Klaus

CORPORATE SOURCE: Department of Chemistry, Carlsberg Laboratory, Copenhagen, DK-2500, Den.

SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1997), (9), 1365-1374
CODEN: JCPRB4; ISSN: 0300-922X

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 09 Jun 1997

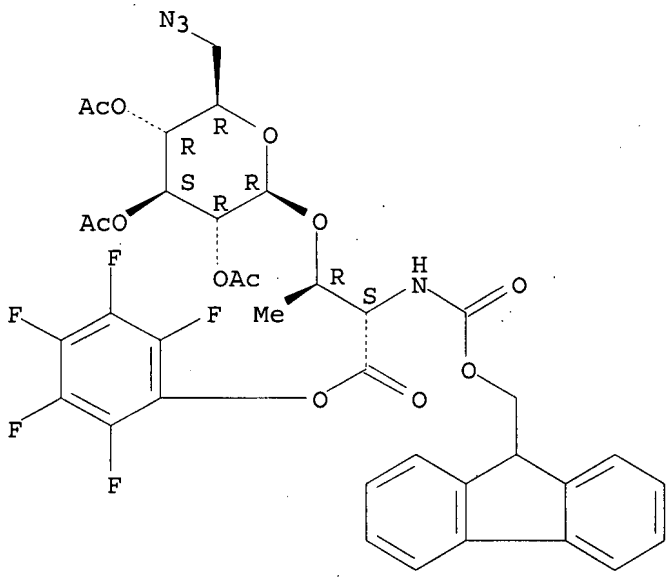
AB A panel of α-helical, dimeric coiled-coil peptides has been designed and synthesized for the evaluation of the effect of glycosylation on the conformation of these coiled-coil peptides. Two glycosylated building blocks, Nα-(fluoren-9-ylmethoxycarbonyl)-O-(2,3,4-tri-O-acetyl-6-azido-6-deoxy-β-D-glucopyranosyl)-L-threonine pentafluorophenyl ester and Nα-(fluoren-9-ylmethoxycarbonyl)-O-{2,3,4-tri-O-acetyl-6-[2'-(tert-butoxycarbonylamino)benzoylamino]-6-deoxy-β-D-glucopyranosyl}-L-threonine pentafluorophenyl ester containing the fluorogenic 2-aminobenzamide (Abz) group, have been synthesized. These compds. have been obtained by the glycosylation of Nα-Fmoc-Thr-OPfp with the corresponding glycosyl trichloroacetamidate donors and have been incorporated into the solid-phase synthesis of the peptides and glycopeptides. Five compds. have been synthesized as internally quenched fluorogenic compds. where the Abz group has been employed as the fluorogenic probe and 3-nitrotyrosine Tyr(NO2) as the quenching chromophore. Steady-state fluorescence studies have provided evidence to support the dimerization of the α-helical peptides. Denaturation studies, by fluorescence as well as CD spectroscopy, indicate that the introduction of a carbohydrate moiety into the coiled-coil peptides has a significant destabilizing effect on the α-helicity.

IT **191668-75-4P 191668-76-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(internally quenched fluorogenic, helical dimeric peptides and glycopeptides for evaluation of effect of glycosylation on conformation of peptides)

RN 191668-75-4 HCAPLUS

CN L-Threonine, N-[(9H-fluoren-9-ylmethoxy)carbonyl]-O-(2,3,4-tri-O-acetyl-6-azido-6-deoxy-β-D-glucopyranosyl)-, pentafluorophenyl ester (9CI) (CA INDEX NAME)

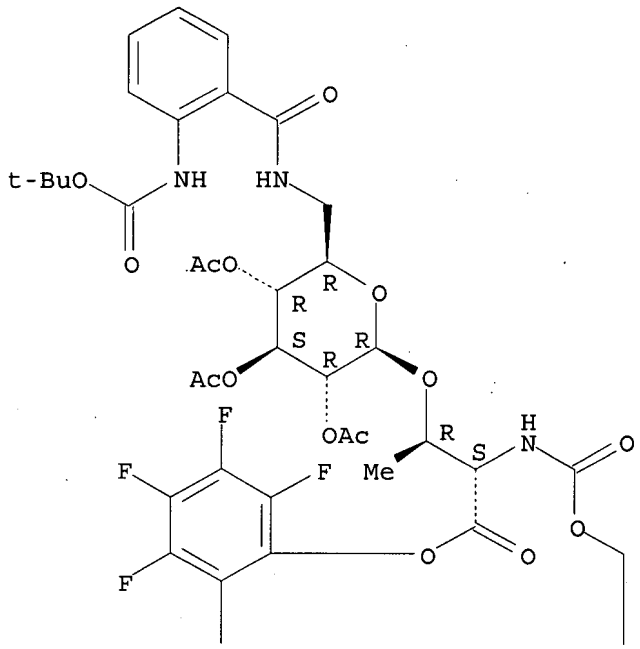
Absolute stereochemistry.



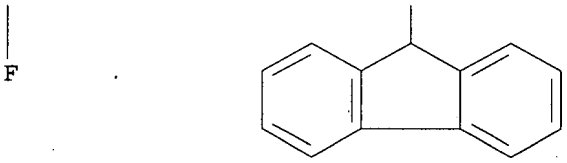
RN 191668-76-5 HCAPLUS
CN L-Threonine, N-[(9H-fluoren-9-ylmethoxy)carbonyl]-O-[2,3,4-tri-O-acetyl-6-deoxy-6-[[2-[[(1,1-dimethylethoxy)carbonyl]amino]benzoyl]amino]-β-D-glucopyranosyl]-, pentafluorophenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-A



PAGE 2-A



REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=>